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N	EWS	3	JAN	06	The retention policy for unread STNmail messages													
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NEWS		4	JAN	07	WPIDS, WPINDEX, and WPIX enhanced Japanese Patent													
					Classification Data													
NI	EWS	5	FEB	02	Simultaneous left and right truncation (SLART) added													
					for CERAB, COMPUAB, ELCOM, and SOLIDSTATE													
	EWS	6	FEB		GENBANK enhanced with SET PLURALS and SET SPELLING													
	EWS	7	FEB		Patent sequence location (PSL) data added to USGENE													
	EWS		FEB		COMPENDEX reloaded and enhanced													
	EWS		FEB		WTEXTILES reloaded and enhanced													
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					patent records provide insights into related prior													
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1 2 3 4 5 6 7 8 9 10 11 12 chain bonds:
5-16 6-13 7-18 10-13 13-15 13-14 16-17 17-20 ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 exact/norm bonds:
13-15 13-14 17-20 exact bonds:
5-16 6-13 7-18 10-13 16-17 normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
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G1:C,H

Match level :

chain nodes :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS

=> d 11 L1 HAS NO ANSWERS

G1 C,H

Structure attributes must be viewed using STN Express query preparation.

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1 2 3 4 5 6 7 8 9 10 11 12 chain bonds:
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13-15 14-22 17-20 exact bonds:
5-16 6-13 7-18 10-13 13-14 16-17 normalized bonds:
13-16 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
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G1:C,H

G2:C,H,O,N,CN

chain nodes :

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 20:CLASS 22:CLASS 22

=> d 12 L2 HAS NO ANSWERS L2 STR

G1 C, H G2 C, H, O, N, CN

Structure attributes must be viewed using STN Express query preparation.

127 ANSWERS

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100.0% PROCESSED 539 ITERATIONS

SEARCH TIME: 00.00.01

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 FULL ESTIMATED COST
 193.08
 193.30

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FILE COVERS 1907 - 14 Apr 2009 VOL 150 ISS 16 FILE LAST UPDATED: 13 Apr 2009 (20090413/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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http://www.cas.org/legal/infopolicy.html

=> s 13

L.4

1.5

L6

This file contains CAS Registry Numbers for easy and accurate substance identification.

68 L3 => s 14 and pd<20040300 24836013 PD<20040300 (PD<20040300) 24 L4 AND PD<20040300 => s 15 and (anhydride or imide or precipitate) 241598 ANHYDRIDE 35581 ANHYDRIDES 253168 ANHYDRIDE (ANHYDRIDE OR ANHYDRIDES) 25820 IMIDE 11104 IMIDES 31613 IMIDE (IMIDE OR IMIDES) 16155 PRECIPITATE 15240 PRECIPITATES 29451 PRECIPITATE (PRECIPITATE OR PRECIPITATES) 208189 PPT 71553 PPTS 259282 PPT (PPT OR PPTS) 277250 PRECIPITATE (PRECIPITATE OR PPT) 4 L5 AND (ANHYDRIDE OR IMIDE OR PRECIPITATE) => d 16 1-4 abs ibib hitstr

ANSWER 1 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN

AB The enzymic resolution of 4-[4-(Dimethylamino)-1-(4-fluorophenyl)-1hydroxybutyl]-3-(hydroxymethyl)benzonitrile, a useful intermediate in the synthesis of enantiomerically pure citalopram, has been studied. Candida antarctica lipase B (CAL-B) catalyzes the enzymic acetylation of the primary benzylic alc. with high enantioselectivity at the quaternary stereogenic center. This enzymic acetylation yielded the acetylated

(+) -3-[(acetyloxy)methyl]-4-[(1R)-4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]benzonitrile and the desired

(-) -4 -[(1S) -4 -(dimethylamino) -1 -(4 -fluorophenyl) -1 -hydroxybutyl] -3

(hydroxymethyl)benzonitrile. The enzymic enantioselective hydrolysis of the 3-acetyloxymethyl derivative catalyzed by CAL-B is also possible.

ACCESSION NUMBER: 2004:40088 CAPLUS

DOCUMENT NUMBER: 140:287145

TITLE: Enzymatic resolution of a quaternary stereogenic

center as the key step in the synthesis of (S)-(+)-citalopram

(S)-(+)-citalopram

AUTHOR(S): Solares, Laura F.; Brieva, Rosario; Quiros, Margarita;

Llorente, Isidro; Bayod, Miguel; Gotor, Vicente
CORPORATE SOURCE: Departamento de Quimica Organica e Inorganica,

Facultad de Quimica, Universidad de Oviedo, Oviedo,

33071, Spain

SOURCE: Tetrahedron: Asymmetry (2004), 15(2),

341-345

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:287145

IT 481047-48-7P

RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP

(Preparation)

(regioselective, chemoselective enzymic acetylation and resolution of [(dimethylamino)(fluorophenyl)(hydroxy)butyl](hydroxymethyl)benzonitril e as key step in synthesis of (S)-(+)-citalopram)

RN 481047-48-7 CAPLUS

Total 4 - Car Loos

Note: The Control of the Contro

Absolute stereochemistry. Rotation (+).

IT 488787-59-3P

RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(regioselective, chemoselective enzymic acetylation and resolution of ((dimethylamino) (fluorophenyl) (hydroxy) butyl) (hydroxymethyl) benzonitril e as key step in synthesis of (S)-(+)-citalopram)

RN 488787-59-3 CAPLUS

CN Benzonitrile, 4-[(1S)-4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]3-(hydroxymethyl)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 674806-13-4P 674806-14-5P

RL: BPN (Biosynthetic preparation); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(regioselective, chemoselective enzymic acetylation and resolution of [(dimethylamino)(fluorophenyl)(hydroxy)butyl](hydroxymethyl)benzonitril e as key step in synthesis of (S)-(+)-citalopram)

RN 674806-13-4 CAPLUS

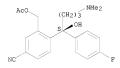
CN Benzonitrile, 3-[(acetyloxy)methyl]-4-[(1R)-4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 674806-14-5 CAPLUS

CN Benzonitrile, 3-[(acetyloxy)methyl]-4-[(1S)-4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



- IT 103146-25-4, 4-[4-(Dimethylamino)-1-(4-fluorophenyl)-1hydroxybutyl]-3-(hydroxymethyl)benzonitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 - (regioselective, chemoselective enzymic acetylation and resolution of [(dimethylamino) (fluorophenyl) (hydroxy)butyl] (hydroxymethyl) benzonitril e as key step in synthesis of (5)-(+)-citalopram)
- RN 103146-25-4 CAPLUS
- CN Benzonitrile, 4-[4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]-3-(hydroxymethyl)- (CA INDEX NAME)

IT 674806-15-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(regioselective, chemoselective enzymic acetylation and resolution of [(dimethylamino)(fluorophenyl)(hydroxy)butyl](hydroxymethyl)benzonitril e as key step in synthesis of (S)-(+)-citalopram)

RN 674806-15-6 CAPLUS

CN Benzonitrile, 3-[(acetyloxy)methyl]-4-[4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]- (CA INDEX NAME)

REFERENCE COUNT: 10

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN GI

AB Preparation of escitalopram (I) via the chiral enriched monoacetate ester of (4-bromo-2-(hydroxymethyl)phenyl)-(4-fluorophenyl)methanol (II) was disclosed. For example, a racemic mixture of monoacetate ester II (13.52 g) and (+)-di-p-toluoyl tartaric acid (11.92 g) in acetone (135 mL) was heated at reflux until a pale brown solution was obtained. The solution was cooled, the acetone removed under vacuum and the resulting brown foam recrystd. from acetone-hexane (2:1) to afford the (+)-di-p-toluoyl tartaric acid salt of monoacetate ester II with a diastereomeric ratio of 97:3. Of note, the claimed (+)-di-p-toluoyl tartaric acid salt of monoacetate ester II was converted to escitalopram oxalate in 4-steps with $[\alpha]D = +10.1^{\circ}$ (at 20°C, c 0.95 in MeOH).

2003:837069 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 139:337880 TITLE: Preparation of escitalopram via the chiral enriched

diol monoesters of

(4-bromo-2-(hydroxymethyl)phenyl)-(4fluorophenyl)methanol

INVENTOR(S): Tse, Hoi Lun Allan PATENT ASSIGNEE(S): Torcan Chemical Ltd., Can.

SOURCE: PCT Int. Appl., 30 pp. CODEN: PIXXD2 Patent

DOCUMENT TYPE: LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

								DATE APPLICATION NO.												
	WO 2003087081																			
		W:	AE.	AG.	AL.	AM.	AT.	AU,	AZ.	BA.	BB.	BG.	BR.	BY.	BZ.	CA.	CH.	CN.		
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(Reactant or reagent)

(intermediate; preparation of escitalopram via a chiral enriched diol monoester intermediate)

RN 488148-10-3 CAPLUS

CN

1,2-Benzenedimethanol, 4-bromo-\alpha1-[3-(dimethylamino)propyl]-\alpha1-(4-fluorophenvl) - (CA INDEX NAME)

RN 488148-12-5 CAPLUS

CN 1,2-Benzenedimethanol, 4-bromo- α 1-[3-(dimethylamino)propyl]- α 1-(4-fluorophenyl)-, (α 1S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 616217-14-2 CAPLUS

CN 1,2-Benzenedimethanol, 4-bromo- α 1-[3-(dimethylamino)propyl]- α 1-(4-fluorophenyl)-, 2-acetate (CA INDEX NAME)

RN 616217-15-3 CAPLUS

CN 1,2-Benzenedimethanol, 4-bromo- α 1-[3-(dimethylamino)propyl]- α 1-(4-fluorophenyl)-, 2-acetate, (α 1S)- (CA INDEX NAME)

Absolute stereochemistry.

RN 616217-16-4 CAPLUS

CN Butanedioic acid, 2,3-bis[(4-methylbenzoyl)oxyl-, (28,38)-, compd. with [5-bromo-2-[(1S)-4-(dimethylamino)-1-(4-fluorophenyl)-1- hydroxybutyl]phenyl]methyl acetate (1:1) (9C1) (CA INDEX NAME)

CM 1

CRN 616217-15-3

CMF C21 H25 Br F N O3

Absolute stereochemistry.

CM 2

CRN 32634-68-7 CMF C20 H18 O8

Absolute stereochemistry. Rotation (+).

REFERENCE COUNT:

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

7 L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN GI

AB This invention relates to the preparation of I and II and derivs. of I and II in their racemic, enantiomerically enriched, or optically pure forms. This invention further relates to novel compns. of matter containing enantiomerically enriched (-)-desmethylcitalopram (-)-III (R = Me), (+)-didesmethylcitalopram (+)-III (R = Me), or (-)-didesmethylcitalopram (-)-III (R = H) or mixts. thereof in optimal ratios. Contrary to prior teachings, the enantiomerically enriched citalopram metabolites disclosed herein possess potent serotonin reuptake inhibitory activity, with minimal inhibitory effects on the reuptake of other known monoamines, e.g., norepinephrine (NE) or dopamine (DA). For example, stepwise reaction of 1-oxo-1,3-dihydroisobenzofuran-5-carbonitrile with 4-fluorophenylmagnesium bromide and the chiral Grignard reagent, which was prepared from 2-(2-bromoethyl)-[1,3]dioxolane and Mg powder, in THF gave II. Cyclization using mesyl chloride in CH2Cl2, followed by reduction provided the I. Reaction of the aldehyde with (-)-tert-butylsulfinamide in the presence of Ti(OEt)4 in EtOH afforded the sulfinamide, which was reduced to the amine III (R = H) with 10% HCl in MeOH. Protection of the amine with BOC anhydride in the presence of TEA in CH2C12 provided the enantiomerically enriched isomers, which were separated on a chiral column and subsequently deprotected with TFA to give (+)-III (R = H) and (-)-III (R = H). In biol. assays, (-)-III (R = H) and (+)-III (R = H) strongly inhibited serotonergic 5-HT receptor activity with Ki values of 5.8 nM and 90 nM, resp., with little effect on NE and DA transporter activity. By comparison, racemic citalopram inhibited serotonin reuptake with a Ki of 3.9 nM. The present invention also discloses methods for treating disorders, dysfunctions and diseases for which inhibition of serotonin reuptake is therapeutically beneficial. In particular, the present invention discloses a method for treating various forms of depression and other CNS disorders with pharmaceutical compns. described herein. ACCESSION NUMBER: 2003:376842 CAPLUS DOCUMENT NUMBER: 138:385297 TITLE: Methods for treating depression and other CNS

disorders using enantiomerically enriched desmethyland didesmethyl- metabolites of citalopram INVENTOR(S): Bush, Larry R.; Currie, Mark G.; Senanayake, Chris H.; Fang, Kevin Q.

PATENT ASSIGNEE(S): Sepracor, Inc., USA
SOURCE: PCT Int. Appl., 58 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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IT 526204-34-2P, 4-[3-([1,3]Dioxolan-2-y1)-1-(4-fluoropheny1)-1hydroxypropy1]-3-hydroxymethylbenzonitrile 526204-42-2P,

(R)-4-[3-([1,3]Dioxolan-2-y1)-1-(4-fluorophenyl)-1-hydroxypropyl]-3-hydroxymethylbenzonitrile

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of enantiomerically enriched desmethyl- and didesmethyl- metabolites of citalopram for treating depression and other CNS disorders)

RN 526204-34-2 CAPLUS

CN Benzonitrile, 4-[3-(1,3-dioxolan-2-y1)-1-(4-fluoropheny1)-1-hydroxypropy1]3-(hydroxymethy1)- (CA INDEX NAME)

- RN 526204-42-2 CAPLUS
- CN Benzonitrile, 4-((1R)-3-(1,3-dioxolan-2-yl)-1-(4-fluorophenyl)-1hydroxypropyl]-3-(hydroxymethyl)- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2009 ACS on STN GI

AB There is described a process for the preparation of citalopram (shown as I) and of its pharmaceutically acceptable salts, which comprises treating a 1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-5-isobenzofurancarbaldoxime, O-substituted preferably with a diphenylmethyl or triphenylmethyl group, with formic-acetic anhydride. Furthermore, the total synthesis of citalopram, as free base or as its pharmaceutically acceptable salt, starting from 5-formylphthalide is described.

ACCESSION NUMBER: 2003:96293 CAPLUS

DOCUMENT NUMBER: 138:137156

TITLE: Process for the preparation of 5-substituted isobenzofurans including citalopram

INVENTOR(S): Dall'asta, Leone; Cotticelli, Giovanni

PATENT ASSIGNEE(S): Infosint SA, Switz.

SOURCE: Eur. Pat. Appl., 22 pp. CODEN: EPXXDW

DOCUMENT TYPE: LANGUAGE: Patent English

KIND DATE

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	TENT :				KIND DATE							D							
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AT	2860	37			T		2005	0115		AT	2001- 2001-	8305	17		21	0010	802		
ES	2234	13		2005	0 / 0 1		ES	2001- 2002-	8305	17		21	0010	802					
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AU	2002	3253	85		A1		2003	0217		AU	2002-	3253	85		2	0020	729	<	
AU	2002	3253	85		B2		2007	0705											
BR	2002	0118	58		A		2004	0921		BR	2002-	1185	20020729						
HU	2004	0011	66		A2		2004	0928		HU	2004-	1166		20020729 20020729 20020729 20020729 20020729					
HU	2004	0011	66		A3		2007	0529											
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CN	1298	713			С		2007	0207											
JP	2005	5010	56		Т		2005	0113		JP	2003-	5170		20020729 20020729 20020731					
RO	1221	47			B1		2009	0130		RO	2004-	84			2	0020	729		
BG	1085	54			A		2005	0331		BG	2004-	1085	54		2	0040	130		
US	2004	0230	065		A1		2004	1118		US	2004- 2004- 2004-	7766	25		2	0040	131		
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MX	2004	0010	30		A		2004	1203		MX	2004-	1030			2	0040	202		
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(process for preparation of 5-substituted isobenzofurans including citalopram)

OTHER SOURCE(S): CASREACT 138:137156; MARPAT 138:137156 IT 493015-02-4P, O-Benzyl-3-hydroxymethyl-4-[a-hydroxy-a-

^{[3-(}dimethylamino)propyl]-4-fluorobenzyl]benzaldoxime 493015-07-9P

[,] O-Triphenylmethyl-3-hydroxymethyl-4-[α -hydroxy- α -[3-

⁽dimethylamino)propyl]-4-fluorobenzyl]benzaldoxime

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

CN Benzaldehyde, 4-[4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]-3-(hydroxymethyl)-, 0-(phenylmethyl)oxime (CA INDEX NAME)

- RN 493015-07-9 CAPLUS
- CN Benzaldehyde, 4-[4-(dimethylamino)-1-(4-fluorophenyl)-1-hydroxybutyl]-3-(hydroxymethyl)-, 0-(triphenylmethyl)oxime (CA INDEX NAME)

- REFERENCE COUNT:
- 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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